New Modeling Strategy for Atom Transfer Radical Polymerization

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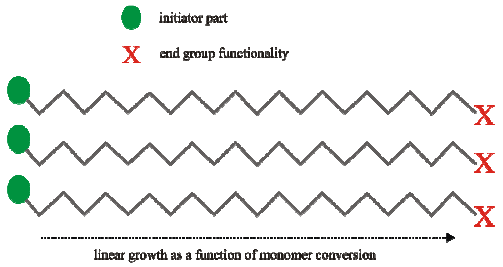
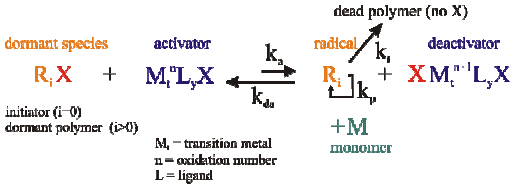
IDECAT Integrated Design of Catalytic Nanomaterials for a Sustainable Production

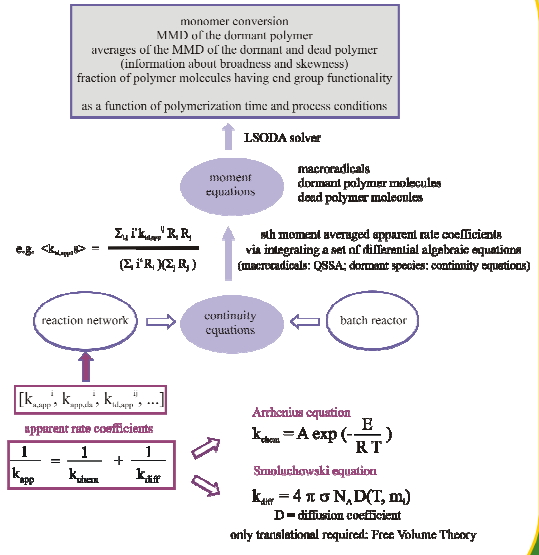
Objectives of ATRP



Reaction mechanism of ATRP

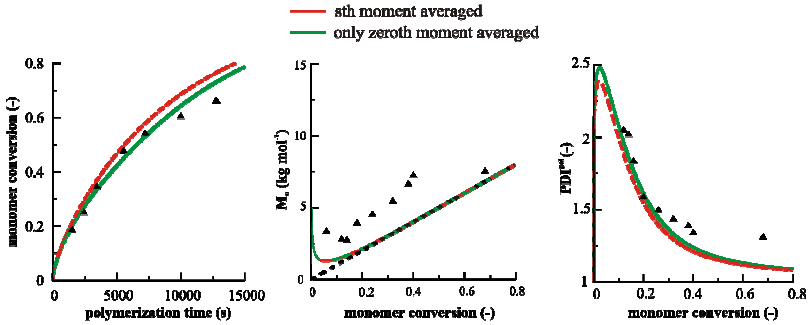


Modeling strategy



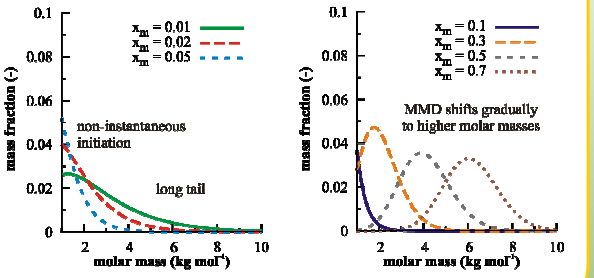
D'hooge et al., **Macromol. React. Eng.**, 20.04.2009, 10.1002/mren.200800051

Comparison with experimental data



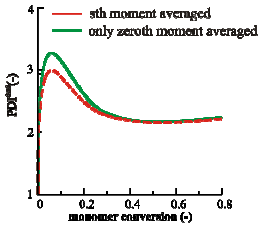
$[MMA]_0 / [R_nX]_0 / [Cu(I)Br]_0 / [PMDETA]_0 = 100/1/0.5/0.5$; $[MMA]_0 = 3100$ mol m^{-3}; $[Cu(II)Br_2] = 0$ mol m^{-3}
polymerization temperature: 363 K; solvent: toluene; MMA: methyl methacrylate; R_nX: ethyl 2-bromo isobutyrate
PMDETA: N,N,N',N'',N''-pentamethyldiethylene-triamine
Experimental data: Snijder et al., **Macromolecules** 2002, *35*, 4785

MMD of the dormant polymer



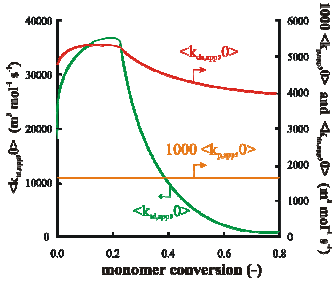
x_m = monomer conversion

Dead polymer



for dead polymer properties accounting for sth moment averaged apparent rate coefficients is important

Diffusional limitations



important for termination and deactivation

Conclusions

The monomer conversion, the MMD of the dormant polymer, averages of the MMD of the dead and dormant polymer are calculated as a function of polymerization time and process conditions, while accounting for diffusional limitations on all reaction steps in a fundamental way. Simulation results are in agreement with experimental data from literature.

Acknowledgments

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